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1-Benzyl-3-(8-methoxyquinolin-2-ylmethyl)imidazolium hexafluoridophosphate

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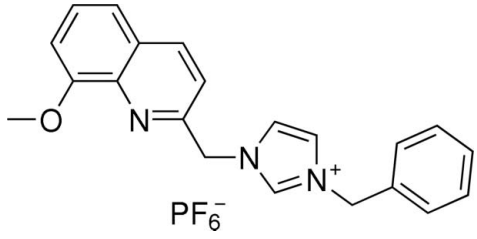
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.008 Å; disorder in solvent or counterion; R factor = 0.065; wR factor = 0.215; data-to-parameter ratio = 11.2.

The asymmetric unit of the title compound, $C_{21}H_{20}N_3O^+\cdot PF_6^-$, contains two independent 1-benzyl-3-(8-methoxyquinolin-2-ylmethyl)imidazolium cationic units and two PF_6^- ions. The two cationic units differ slightly in the orientations of the benzylimidazolium group with respect to the quinoline ring system. In one of the cationic units, the quinoline ring system and the phenyl ring form dihedral angles of 76.0 (1) and 73.8 (1)°, respectively, with the central five-membered ring, and in the other unit these angles are 85.6 (1) and 69.0 (2)°, respectively. Both hexafluoridophosphate ions are found to be disordered over two positions, with site occupancies of *ca* 0.74 and 0.26. The crystal packing is stabilized by C—H···F and C—H···N hydrogen bonds.

Related literature

For general background, see: Herrmann (2002); Herrmann & Kocher (1997). For synthesis, see: Lee *et al.* (2004).



Experimental

Crystal data

$C_{21}H_{20}N_3O^+\cdot F_6P^-$
M_r = 475.37
Triclinic, $P\overline{1}$
a = 12.272 (3) Å
b = 12.537 (3) Å
c = 14.361 (3) Å
α = 90.847 (3)°
β = 91.539 (3)°
γ = 93.809 (3)°
V = 2203.5 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 291 (2) K
0.49 × 0.45 × 0.43 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.911, T_{max} = 0.922
15491 measured reflections
7961 independent reflections
4602 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.215
S = 1.05
7961 reflections
708 parameters
240 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11B···F6^{i}	0.97	2.53	3.071 (7)	115
C12—H12···F9^{ii}	0.93	2.53	3.403 (11)	157
C13—H13···F9^{iii}	0.93	2.42	3.341 (11)	173
C14—H14···N1^{i}	0.93	2.38	3.248 (5)	156
C15—H15A···F11^{iii}	0.97	2.39	3.314 (8)	159
C35—H35···N6^{iv}	0.93	2.42	3.343 (5)	174
C36—H36A···F8^{v}	0.97	2.52	3.217 (8)	129

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x+1, y, z$; (iii) $-x+1, -y+1, -z$; (iv) $-x+1, -y, -z+2$; (v) $-x+1, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL97*.

Many thanks are expressed to the Department of Pharmacy of Gannan Medical University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2422).

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supplementary materials

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1-Benzyl-3-(8-methoxyquinolin-2-ylmethyl)imidazolium hexafluoridophosphate

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Comment

Numerous flexible and rigid N-heterocyclic carbene precursors have been synthesized and studied. They have attracted considerable attention because of their diverse coordination capabilities and the important catalytic properties of their metal complexes (Herrmann, 2002; Herrmann & Kocher, 1997). We report here the crystal structure of the title compound.

The asymmetric unit of the title compound contains two independent $[C_{21}H_{20}N_3O]^+$ cationic units and two PF_6^- ions (Fig. 1). The two cationic units differ in the orientations of the benzylimidazolium group with respect to the quinoline ring system. Bond lengths and angles in the title compound show normal values. The quinoline ring system in each independent molecule is planar.

The N1/C1–C9 and C16–C21 planes form dihedral angles of 76.0 (1)° and 73.8 (1)°, respectively, with the N2/N3/C12–C14 plane. The N6/C22–C30 and C37–C42 planes form dihedral angles of 85.6 (1)° and 69.0 (2)°, respectively, with the N2/N3/C12–C14 plane.

As can be seen from Fig. 2, the hexafluorophosphate ions are linked to 1-benzyl-3-(2-methylene-8-methoxy-quinoline)imidazolium ions through C—H···F hydrogen bonds (Table 1). A C—H···N hydrogen bond is also observed.

Experimental

The title compound was synthesized by the reaction of 2-bromomethyl-8-methoxy-quinoline (0.25 g) with 1-benzyl-1*H*-imidazole (0.2 g) in tetrahydrofuran at 350 K, according to a literature method (Lee *et al.*, 2004). A white precipitate was obtained, and it was dissolved in methol (5 ml) and then ammonium hexafluorophosphate (0.2 g) was added. The resulting solid was filtered off, washed with ethyl ether and air-dried. White single crystals suitable for X-ray diffraction were obtained by recrystallization from absolute acetionitrile and ethyl ether (1:2).

Refinement

Both hexafluorophosphate ions were found to be disordered over two positions, with refined site occupancies of 0.742 (10) and 0.258 (10) [P1,F1–F6/P1',F1'–F6'] or 0.739 (19) and 0.261 (19) [P2,F7–F12/P2',F2'–F12']. The P—F and F···F distances were restrained to 1.57 (1) and 2.21 (2) Å, and the displacement parameters of all disordered atoms were restrained to an approximate isotropic behaviour. H atoms were positioned geometrically, with C—H = 0.93, 0.96 and 0.97 Å for aromatic, methyl and methylene H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

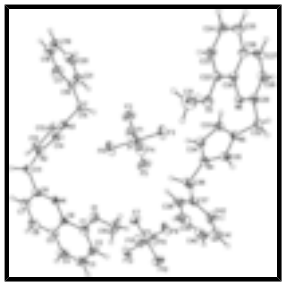


Fig. 1. The asymmetric unit of the title compound, showing 30% probability displacement ellipsoids and the atomic numbering. Only the major disorder component is shown.

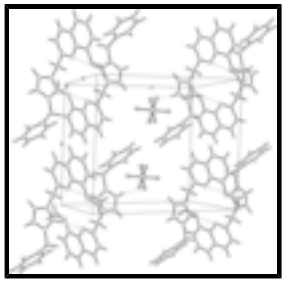


Fig. 2. The crystal of the packing of the title compound, viewed along the *a* axis. C—H···F and C—H···N hydrogen bonds are shown as dashed lines. Only the major disorder component is shown.

1-Benzyl-3-(8-methoxyquinolin-2-ylmethyl)imidazolium hexafluoridophosphate

Crystal data

$C_{21}H_{20}N_3O^+·F_6P^-$	$Z = 4$
$M_r = 475.37$	$F_{000} = 976$
Triclinic, $P\bar{1}$	$D_x = 1.433$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 12.272$ (3) Å	Cell parameters from 2858 reflections
$b = 12.537$ (3) Å	$\theta = 2.7$–23.6º
$c = 14.361$ (3) Å	$\mu = 0.19$ mm^{-1}
$\alpha = 90.847$ (3)º	$T = 291$ (2) K
$\beta = 91.539$ (3)º	Block, white
$\gamma = 93.809$ (3)º	0.49 × 0.45 × 0.43 mm
$V = 2203.5$ (8) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	7961 independent reflections
Radiation source: fine-focus sealed tube	4602 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.038$
$T = 291(2)$ K	$\theta_{max} = 25.5$º
φ and ω scans	$\theta_{min} = 2.4$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1997)	$h = -14 \rightarrow 14$
$T_{min} = 0.911$, $T_{max} = 0.922$	$k = -15 \rightarrow 15$

15491 measured reflections

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.065$

$wR(F^2) = 0.215$

$S = 1.05$

7961 reflections

708 parameters

240 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0928P)^2 + 1.4093P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.50$ e Å^{-3}

$\Delta\rho_{min} = -0.24$ e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0057 (11)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
P1	0.6866 (3)	0.2339 (3)	0.4728 (3)	0.0605 (19)	0.742 (10)
F1	0.6701 (4)	0.2242 (6)	0.3625 (3)	0.109 (2)	0.742 (10)
F2	0.7707 (5)	0.1462 (5)	0.4689 (5)	0.124 (2)	0.742 (10)
F3	0.5890 (6)	0.1459 (6)	0.4837 (5)	0.111 (2)	0.742 (10)
F4	0.7030 (4)	0.2430 (5)	0.5810 (3)	0.104 (2)	0.742 (10)
F5	0.6003 (5)	0.3196 (5)	0.4755 (5)	0.135 (3)	0.742 (10)
F6	0.7822 (5)	0.3205 (5)	0.4588 (4)	0.109 (2)	0.742 (10)
P1'	0.6893 (9)	0.2309 (9)	0.4643 (8)	0.063 (6)	0.258 (10)
F1'	0.7114 (11)	0.1534 (11)	0.3811 (10)	0.090 (5)	0.258 (10)
F2'	0.7923 (13)	0.1921 (16)	0.5154 (13)	0.158 (9)	0.258 (10)
F3'	0.6187 (16)	0.1361 (14)	0.5069 (14)	0.124 (9)	0.258 (10)
F4'	0.6676 (14)	0.3058 (15)	0.5485 (13)	0.140 (7)	0.258 (10)
F5'	0.5902 (10)	0.2719 (14)	0.4092 (13)	0.128 (7)	0.258 (10)
F6'	0.7659 (12)	0.3220 (10)	0.4227 (13)	0.094 (6)	0.258 (10)
P2	0.1795 (4)	0.7468 (4)	0.0546 (3)	0.0571 (12)	0.739 (19)

F7	0.2725 (6)	0.6773 (5)	0.0189 (7)	0.110 (3)	0.739 (19)
F8	0.1989 (5)	0.7013 (7)	0.1553 (4)	0.090 (2)	0.739 (19)
F9	0.0912 (8)	0.6513 (7)	0.0333 (7)	0.114 (3)	0.739 (19)
F10	0.0869 (6)	0.8149 (7)	0.0922 (7)	0.130 (3)	0.739 (19)
F11	0.1606 (9)	0.7891 (6)	−0.0466 (4)	0.116 (3)	0.739 (19)
F12	0.2675 (6)	0.8413 (6)	0.0764 (6)	0.092 (2)	0.739 (19)
P2'	0.1689 (11)	0.7337 (12)	0.0456 (10)	0.067 (5)	0.261 (19)
F7'	0.2338 (19)	0.6744 (15)	−0.0290 (19)	0.129 (8)	0.261 (19)
F8'	0.2211 (17)	0.6680 (15)	0.1248 (17)	0.101 (7)	0.261 (19)
F9'	0.0738 (13)	0.6427 (13)	0.0332 (13)	0.062 (5)	0.261 (19)
F10'	0.1024 (19)	0.7933 (17)	0.1193 (12)	0.113 (7)	0.261 (19)
F11'	0.1105 (19)	0.7986 (15)	−0.0311 (12)	0.104 (7)	0.261 (19)
F12'	0.2669 (16)	0.8208 (16)	0.0533 (18)	0.109 (9)	0.261 (19)
O1	0.7717 (3)	0.6213 (3)	0.5771 (3)	0.0933 (11)	
O2	0.7504 (2)	−0.1017 (2)	1.0211 (2)	0.0746 (9)	
N1	0.9222 (3)	0.6509 (3)	0.4472 (2)	0.0546 (8)	
N2	1.0364 (3)	0.4949 (3)	0.3131 (2)	0.0541 (8)	
N3	0.9645 (3)	0.3409 (3)	0.2674 (2)	0.0564 (9)	
N4	0.5105 (3)	0.1467 (3)	0.7904 (3)	0.0608 (9)	
N5	0.4442 (2)	−0.0133 (3)	0.8162 (2)	0.0520 (8)	
N6	0.5660 (3)	−0.1618 (2)	0.9259 (2)	0.0508 (8)	
C1	0.7622 (4)	0.7075 (4)	0.5216 (4)	0.0701 (12)	
C2	0.6811 (4)	0.7791 (5)	0.5282 (4)	0.0916 (17)	
H2	0.6277	0.7697	0.5726	0.110*	
C3	0.6800 (5)	0.8665 (5)	0.4669 (5)	0.103 (2)	
H3	0.6248	0.9136	0.4713	0.124*	
C4	0.7548 (5)	0.8831 (4)	0.4037 (5)	0.0972 (18)	
H4	0.7527	0.9422	0.3655	0.117*	
C5	0.8392 (4)	0.8110 (4)	0.3936 (3)	0.0713 (13)	
C6	0.9207 (5)	0.8250 (4)	0.3281 (3)	0.0872 (16)	
H6	0.9211	0.8825	0.2879	0.105*	
C7	1.0005 (5)	0.7529 (4)	0.3233 (3)	0.0805 (14)	
H7	1.0561	0.7618	0.2808	0.097*	
C8	0.9964 (3)	0.6664 (3)	0.3835 (3)	0.0577 (10)	
C9	0.8432 (3)	0.7221 (3)	0.4532 (3)	0.0580 (10)	
C10	0.6958 (6)	0.6066 (7)	0.6503 (6)	0.170 (4)	
H10A	0.7016	0.6682	0.6910	0.255*	
H10B	0.7120	0.5444	0.6850	0.255*	
H10C	0.6230	0.5972	0.6241	0.255*	
C11	1.0793 (4)	0.5831 (3)	0.3756 (3)	0.0650 (12)	
H11A	1.1465	0.6154	0.3513	0.078*	
H11B	1.0956	0.5554	0.4368	0.078*	
C12	1.0219 (4)	0.4975 (4)	0.2186 (3)	0.0746 (14)	
H12	1.0397	0.5553	0.1808	0.090*	
C13	0.9773 (4)	0.4018 (4)	0.1901 (3)	0.0714 (13)	
H13	0.9586	0.3808	0.1291	0.086*	
C14	1.0005 (3)	0.3990 (3)	0.3407 (3)	0.0561 (10)	
H14	1.0007	0.3761	0.4020	0.067*	
C15	0.9222 (4)	0.2273 (4)	0.2682 (3)	0.0706 (12)	

H15A	0.8832	0.2097	0.2098	0.085*
H15B	0.8708	0.2177	0.3181	0.085*
C16	1.0119 (4)	0.1517 (3)	0.2818 (3)	0.0630 (11)
C17	1.0769 (5)	0.1275 (4)	0.2090 (4)	0.0953 (18)
H17	1.0663	0.1589	0.1515	0.114*
C18	1.1584 (6)	0.0565 (5)	0.2203 (6)	0.118 (2)
H18	1.2016	0.0392	0.1708	0.142*
C19	1.1735 (5)	0.0125 (5)	0.3066 (7)	0.114 (2)
H19	1.2296	−0.0328	0.3166	0.137*
C20	1.1069 (6)	0.0351 (5)	0.3772 (5)	0.1038 (19)
H20	1.1157	0.0023	0.4343	0.125*
C21	1.0275 (5)	0.1047 (4)	0.3660 (3)	0.0823 (15)
H21	0.9838	0.1205	0.4156	0.099*
C22	0.7408 (3)	−0.2053 (3)	0.9897 (3)	0.0575 (11)
C23	0.8181 (4)	−0.2779 (4)	1.0050 (3)	0.0728 (13)
H23	0.8827	−0.2575	1.0378	0.087*
C24	0.7988 (5)	−0.3843 (4)	0.9703 (4)	0.0889 (18)
H24	0.8512	−0.4333	0.9809	0.107*
C25	0.7063 (5)	−0.4156 (4)	0.9225 (4)	0.0896 (17)
H25	0.6950	−0.4860	0.9010	0.108*
C26	0.6255 (4)	−0.3418 (3)	0.9046 (3)	0.0672 (12)
C27	0.5275 (5)	−0.3680 (4)	0.8540 (4)	0.0865 (16)
H27	0.5131	−0.4372	0.8304	0.104*
C28	0.4540 (4)	−0.2938 (4)	0.8392 (4)	0.0763 (13)
H28	0.3903	−0.3106	0.8040	0.092*
C29	0.4759 (4)	−0.1903 (3)	0.8782 (3)	0.0554 (10)
C30	0.6423 (3)	−0.2354 (3)	0.9388 (3)	0.0525 (10)
C31	0.8499 (5)	−0.0659 (5)	1.0692 (5)	0.109 (2)
H31A	0.8569	−0.1047	1.1259	0.164*
H31B	0.8490	0.0091	1.0834	0.164*
H31C	0.9106	−0.0780	1.0305	0.164*
C32	0.3959 (3)	−0.1062 (3)	0.8645 (3)	0.0663 (12)
H32A	0.3329	−0.1364	0.8286	0.080*
H32B	0.3710	−0.0834	0.9247	0.080*
C33	0.4784 (4)	−0.0108 (4)	0.7262 (3)	0.0686 (13)
H33	0.4739	−0.0678	0.6838	0.082*
C34	0.5190 (4)	0.0879 (4)	0.7103 (3)	0.0719 (13)
H34	0.5480	0.1125	0.6548	0.086*
C35	0.4652 (3)	0.0829 (3)	0.8536 (3)	0.0566 (10)
H35	0.4507	0.1028	0.9144	0.068*
C36	0.5422 (4)	0.2627 (4)	0.8036 (4)	0.0841 (15)
H36A	0.6111	0.2791	0.7736	0.101*
H36B	0.5534	0.2784	0.8696	0.101*
C37	0.4588 (4)	0.3331 (3)	0.7649 (3)	0.0614 (11)
C38	0.4690 (5)	0.3775 (4)	0.6792 (4)	0.0932 (18)
H38	0.5280	0.3625	0.6431	0.112*
C39	0.3919 (7)	0.4451 (5)	0.6449 (4)	0.110 (2)
H39	0.3993	0.4748	0.5863	0.132*
C40	0.3081 (6)	0.4664 (5)	0.6967 (6)	0.103 (2)

H40	0.2564	0.5108	0.6734	0.123*
C41	0.2958 (5)	0.4252 (5)	0.7827 (6)	0.119 (2)
H41	0.2375	0.4421	0.8190	0.143*
C42	0.3715 (4)	0.3580 (5)	0.8149 (4)	0.0934 (17)
H42	0.3626	0.3282	0.8734	0.112*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.057 (3)	0.065 (3)	0.059 (2)	−0.001 (2)	0.0093 (17)	−0.0002 (16)
F1	0.114 (4)	0.147 (5)	0.062 (2)	−0.018 (4)	−0.008 (2)	0.005 (3)
F2	0.131 (4)	0.106 (4)	0.144 (5)	0.056 (3)	0.035 (4)	0.025 (4)
F3	0.094 (4)	0.131 (5)	0.103 (4)	−0.043 (3)	0.015 (3)	0.005 (3)
F4	0.114 (4)	0.135 (4)	0.060 (2)	−0.021 (3)	0.006 (2)	0.011 (2)
F5	0.140 (4)	0.127 (4)	0.150 (5)	0.069 (4)	0.036 (4)	0.015 (4)
F6	0.122 (4)	0.127 (4)	0.067 (3)	−0.067 (3)	0.002 (3)	−0.002 (3)
P1'	0.072 (9)	0.063 (8)	0.054 (6)	0.013 (6)	0.002 (5)	0.009 (5)
F1'	0.086 (8)	0.084 (8)	0.097 (8)	−0.027 (6)	0.017 (6)	−0.030 (6)
F2'	0.146 (11)	0.170 (12)	0.159 (12)	0.046 (9)	−0.063 (9)	−0.017 (9)
F3'	0.151 (13)	0.113 (11)	0.106 (11)	−0.030 (8)	0.021 (8)	0.032 (8)
F4'	0.143 (10)	0.151 (11)	0.127 (10)	0.026 (8)	0.014 (8)	−0.064 (8)
F5'	0.099 (9)	0.141 (10)	0.148 (11)	0.039 (7)	−0.023 (8)	0.008 (8)
F6'	0.104 (9)	0.075 (8)	0.108 (10)	0.019 (7)	0.033 (7)	0.012 (7)
P2	0.055 (2)	0.063 (2)	0.0525 (15)	−0.0003 (15)	−0.0028 (13)	0.0094 (13)
F7	0.102 (4)	0.113 (4)	0.117 (5)	0.028 (3)	0.024 (4)	−0.017 (3)
F8	0.073 (3)	0.133 (5)	0.062 (3)	−0.014 (3)	−0.004 (2)	0.025 (3)
F9	0.116 (5)	0.110 (5)	0.106 (5)	−0.053 (4)	−0.029 (4)	0.017 (4)
F10	0.091 (4)	0.149 (5)	0.156 (6)	0.054 (4)	−0.023 (4)	−0.023 (4)
F11	0.137 (6)	0.118 (5)	0.086 (3)	−0.031 (4)	−0.036 (3)	0.047 (3)
F12	0.101 (4)	0.068 (3)	0.101 (4)	−0.019 (3)	−0.029 (3)	0.005 (3)
P2'	0.077 (8)	0.054 (6)	0.069 (6)	0.008 (5)	−0.020 (4)	0.000 (4)
F7'	0.117 (10)	0.140 (10)	0.132 (11)	0.026 (8)	0.026 (8)	−0.028 (8)
F8'	0.092 (9)	0.085 (9)	0.123 (11)	−0.002 (7)	−0.031 (8)	0.022 (8)
F9'	0.063 (8)	0.063 (8)	0.060 (8)	−0.002 (6)	−0.013 (6)	0.014 (6)
F10'	0.135 (12)	0.133 (11)	0.076 (8)	0.033 (8)	0.026 (7)	−0.017 (7)
F11'	0.105 (10)	0.102 (9)	0.105 (9)	0.013 (8)	−0.028 (7)	0.023 (7)
F12'	0.109 (12)	0.115 (12)	0.097 (11)	−0.039 (8)	−0.002 (7)	0.027 (8)
O1	0.072 (2)	0.101 (3)	0.110 (3)	0.013 (2)	0.030 (2)	0.022 (2)
O2	0.0577 (19)	0.063 (2)	0.102 (2)	0.0048 (16)	−0.0140 (17)	−0.0068 (17)
N1	0.055 (2)	0.051 (2)	0.0564 (18)	0.0001 (16)	−0.0056 (16)	−0.0050 (15)
N2	0.056 (2)	0.059 (2)	0.0463 (17)	0.0007 (17)	0.0026 (15)	−0.0092 (15)
N3	0.059 (2)	0.057 (2)	0.0531 (19)	0.0007 (17)	0.0041 (16)	−0.0035 (16)
N4	0.050 (2)	0.049 (2)	0.082 (2)	0.0018 (17)	−0.0129 (18)	0.0037 (18)
N5	0.0478 (19)	0.050 (2)	0.0583 (19)	0.0068 (16)	−0.0031 (15)	0.0049 (15)
N6	0.055 (2)	0.0427 (18)	0.0558 (18)	0.0048 (16)	0.0052 (16)	0.0068 (14)
C1	0.056 (3)	0.066 (3)	0.088 (3)	0.006 (2)	−0.009 (2)	−0.002 (3)
C2	0.058 (3)	0.096 (4)	0.121 (5)	0.016 (3)	−0.004 (3)	−0.021 (4)
C3	0.089 (4)	0.084 (4)	0.139 (6)	0.037 (4)	−0.021 (4)	−0.020 (4)

C4	0.108 (5)	0.066 (4)	0.119 (5)	0.029 (3)	−0.027 (4)	0.004 (3)
C5	0.089 (4)	0.050 (3)	0.073 (3)	0.007 (2)	−0.019 (3)	−0.006 (2)
C6	0.127 (5)	0.067 (3)	0.067 (3)	0.000 (3)	−0.012 (3)	0.010 (2)
C7	0.105 (4)	0.072 (3)	0.064 (3)	−0.004 (3)	0.009 (3)	0.000 (2)
C8	0.067 (3)	0.054 (3)	0.051 (2)	−0.002 (2)	−0.008 (2)	−0.0080 (19)
C9	0.060 (3)	0.048 (2)	0.064 (2)	0.001 (2)	−0.013 (2)	−0.0110 (19)
C10	0.126 (6)	0.206 (9)	0.191 (8)	0.042 (6)	0.094 (6)	0.081 (7)
C11	0.060 (3)	0.070 (3)	0.063 (3)	0.000 (2)	−0.003 (2)	−0.016 (2)
C12	0.104 (4)	0.066 (3)	0.053 (2)	−0.004 (3)	0.013 (2)	0.006 (2)
C13	0.104 (4)	0.065 (3)	0.044 (2)	−0.003 (3)	0.001 (2)	−0.001 (2)
C14	0.061 (3)	0.061 (3)	0.047 (2)	0.004 (2)	0.0070 (19)	0.0032 (19)
C15	0.066 (3)	0.064 (3)	0.080 (3)	−0.009 (2)	0.003 (2)	0.000 (2)
C16	0.074 (3)	0.052 (3)	0.062 (2)	−0.008 (2)	0.005 (2)	0.000 (2)
C17	0.124 (5)	0.089 (4)	0.077 (3)	0.028 (4)	0.033 (3)	0.013 (3)
C18	0.125 (5)	0.093 (5)	0.141 (6)	0.021 (4)	0.048 (5)	0.007 (4)
C19	0.086 (4)	0.073 (4)	0.184 (8)	0.009 (3)	−0.006 (5)	0.021 (5)
C20	0.119 (5)	0.083 (4)	0.107 (5)	−0.005 (4)	−0.028 (4)	0.024 (3)
C21	0.113 (4)	0.065 (3)	0.068 (3)	−0.005 (3)	−0.002 (3)	0.005 (2)
C22	0.056 (3)	0.055 (3)	0.063 (2)	0.009 (2)	0.007 (2)	0.012 (2)
C23	0.058 (3)	0.081 (3)	0.083 (3)	0.018 (3)	0.006 (2)	0.022 (3)
C24	0.093 (4)	0.076 (4)	0.105 (4)	0.046 (3)	0.019 (3)	0.022 (3)
C25	0.109 (5)	0.057 (3)	0.107 (4)	0.032 (3)	0.009 (4)	−0.002 (3)
C26	0.085 (3)	0.050 (3)	0.069 (3)	0.018 (2)	0.006 (2)	−0.001 (2)
C27	0.117 (5)	0.054 (3)	0.088 (3)	0.006 (3)	−0.004 (3)	−0.019 (3)
C28	0.080 (3)	0.063 (3)	0.085 (3)	0.002 (3)	−0.012 (3)	−0.004 (3)
C29	0.055 (3)	0.054 (3)	0.057 (2)	−0.001 (2)	0.001 (2)	0.0095 (19)
C30	0.060 (3)	0.048 (2)	0.051 (2)	0.009 (2)	0.0112 (19)	0.0060 (17)
C31	0.086 (4)	0.099 (5)	0.139 (5)	0.004 (4)	−0.045 (4)	−0.015 (4)
C32	0.051 (3)	0.068 (3)	0.081 (3)	0.004 (2)	0.000 (2)	0.024 (2)
C33	0.097 (4)	0.061 (3)	0.050 (2)	0.015 (3)	0.003 (2)	−0.002 (2)
C34	0.083 (3)	0.066 (3)	0.069 (3)	0.013 (3)	0.014 (2)	0.015 (2)
C35	0.058 (3)	0.054 (3)	0.059 (2)	0.013 (2)	−0.0071 (19)	−0.002 (2)
C36	0.072 (3)	0.054 (3)	0.123 (4)	−0.004 (3)	−0.028 (3)	−0.001 (3)
C37	0.058 (3)	0.043 (2)	0.082 (3)	−0.005 (2)	−0.008 (2)	0.002 (2)
C38	0.135 (5)	0.069 (3)	0.077 (3)	0.012 (3)	0.026 (3)	−0.005 (3)
C39	0.188 (7)	0.067 (4)	0.075 (4)	0.014 (4)	−0.013 (4)	0.012 (3)
C40	0.104 (5)	0.064 (4)	0.137 (6)	0.003 (3)	−0.053 (4)	0.009 (4)
C41	0.090 (4)	0.114 (5)	0.160 (6)	0.033 (4)	0.023 (4)	0.058 (5)
C42	0.084 (4)	0.099 (4)	0.100 (4)	0.013 (3)	0.016 (3)	0.042 (3)

Geometric parameters (Å, °)

P1—F2	1.559 (5)	C10—H10B	0.96
P1—F5	1.559 (5)	C10—H10C	0.96
P1—F4	1.563 (5)	C11—H11A	0.97
P1—F6	1.564 (5)	C11—H11B	0.97
P1—F3	1.586 (5)	C12—C13	1.339 (6)
P1—F1	1.592 (5)	C12—H12	0.93
P1'—F2'	1.554 (9)	C13—H13	0.93

P1'—F5'	1.554 (9)	C14—H14	0.93
P1'—F4'	1.559 (9)	C15—C16	1.510 (6)
P1'—F6'	1.566 (9)	C15—H15A	0.97
P1'—F3'	1.566 (10)	C15—H15B	0.97
P1'—F1'	1.569 (9)	C16—C21	1.367 (6)
P2—F10	1.569 (5)	C16—C17	1.375 (6)
P2—F12	1.571 (6)	C17—C18	1.389 (8)
P2—F11	1.572 (5)	C17—H17	0.93
P2—F7	1.573 (5)	C18—C19	1.378 (10)
P2—F8	1.580 (5)	C18—H18	0.93
P2—F9	1.581 (6)	C19—C20	1.358 (9)
P2'—F7'	1.561 (9)	C19—H19	0.93
P2'—F8'	1.563 (9)	C20—C21	1.359 (8)
P2'—F10'	1.565 (9)	C20—H20	0.93
P2'—F11'	1.565 (9)	C21—H21	0.93
P2'—F12'	1.570 (10)	C22—C23	1.373 (6)
P2'—F9'	1.581 (10)	C22—C30	1.421 (6)
O1—C1	1.361 (6)	C23—C24	1.420 (7)
O1—C10	1.429 (6)	C23—H23	0.93
O2—C22	1.365 (5)	C24—C25	1.344 (8)
O2—C31	1.428 (6)	C24—H24	0.93
N1—C8	1.316 (5)	C25—C26	1.422 (6)
N1—C9	1.364 (5)	C25—H25	0.93
N2—C14	1.323 (5)	C26—C27	1.405 (7)
N2—C12	1.365 (5)	C26—C30	1.415 (6)
N2—C11	1.474 (5)	C27—C28	1.354 (7)
N3—C14	1.321 (5)	C27—H27	0.93
N3—C13	1.362 (5)	C28—C29	1.411 (6)
N3—C15	1.483 (5)	C28—H28	0.93
N4—C35	1.326 (5)	C29—C32	1.500 (5)
N4—C34	1.368 (6)	C31—H31A	0.96
N4—C36	1.489 (6)	C31—H31B	0.96
N5—C35	1.319 (5)	C31—H31C	0.96
N5—C33	1.370 (5)	C32—H32A	0.97
N5—C32	1.464 (5)	C32—H32B	0.97
N6—C29	1.312 (5)	C33—C34	1.328 (6)
N6—C30	1.370 (5)	C33—H33	0.93
C1—C2	1.388 (6)	C34—H34	0.93
C1—C9	1.421 (6)	C35—H35	0.93
C2—C3	1.417 (8)	C36—C37	1.496 (6)
C2—H2	0.93	C36—H36A	0.97
C3—C4	1.316 (8)	C36—H36B	0.97
C3—H3	0.93	C37—C42	1.357 (6)
C4—C5	1.427 (7)	C37—C38	1.363 (7)
C4—H4	0.93	C38—C39	1.396 (8)
C5—C6	1.396 (7)	C38—H38	0.93
C5—C9	1.419 (6)	C39—C40	1.324 (9)
C6—C7	1.379 (7)	C39—H39	0.93
C6—H6	0.93	C40—C41	1.355 (9)

C7—C8	1.396 (6)	C40—H40	0.93
C7—H7	0.93	C41—C42	1.371 (7)
C8—C11	1.510 (5)	C41—H41	0.93
C10—H10A	0.96	C42—H42	0.93
F2—P1—F5	178.6 (5)	N2—C11—H11A	109.6
F2—P1—F4	90.3 (4)	C8—C11—H11A	109.6
F5—P1—F4	90.4 (4)	N2—C11—H11B	109.6
F2—P1—F6	89.0 (4)	C8—C11—H11B	109.6
F5—P1—F6	92.3 (4)	H11A—C11—H11B	108.1
F4—P1—F6	91.1 (3)	C13—C12—N2	107.7 (4)
F2—P1—F3	91.1 (4)	C13—C12—H12	126.2
F5—P1—F3	87.6 (4)	N2—C12—H12	126.2
F4—P1—F3	90.6 (4)	C12—C13—N3	107.1 (4)
F6—P1—F3	178.3 (5)	C12—C13—H13	126.4
F2—P1—F1	89.4 (4)	N3—C13—H13	126.4
F5—P1—F1	89.9 (4)	N3—C14—N2	109.2 (3)
F4—P1—F1	179.8 (5)	N3—C14—H14	125.4
F6—P1—F1	89.0 (3)	N2—C14—H14	125.4
F3—P1—F1	89.4 (4)	N3—C15—C16	112.6 (4)
F2'—P1'—F5'	177.1 (11)	N3—C15—H15A	109.1
F2'—P1'—F4'	90.7 (9)	C16—C15—H15A	109.1
F5'—P1'—F4'	90.7 (8)	N3—C15—H15B	109.1
F2'—P1'—F6'	87.3 (8)	C16—C15—H15B	109.1
F5'—P1'—F6'	90.1 (8)	H15A—C15—H15B	107.8
F4'—P1'—F6'	89.6 (8)	C21—C16—C17	119.4 (5)
F2'—P1'—F3'	89.6 (9)	C21—C16—C15	120.3 (4)
F5'—P1'—F3'	92.9 (9)	C17—C16—C15	120.3 (4)
F4'—P1'—F3'	91.5 (9)	C16—C17—C18	120.8 (5)
F6'—P1'—F3'	176.7 (10)	C16—C17—H17	119.6
F2'—P1'—F1'	88.5 (8)	C18—C17—H17	119.6
F5'—P1'—F1'	90.1 (8)	C19—C18—C17	118.4 (6)
F4'—P1'—F1'	178.7 (10)	C19—C18—H18	120.8
F6'—P1'—F1'	91.3 (8)	C17—C18—H18	120.8
F3'—P1'—F1'	87.5 (9)	C20—C19—C18	120.2 (6)
F10—P2—F12	90.9 (4)	C20—C19—H19	119.9
F10—P2—F11	91.0 (4)	C18—C19—H19	119.9
F12—P2—F11	90.7 (4)	C19—C20—C21	121.2 (6)
F10—P2—F7	178.8 (5)	C19—C20—H20	119.4
F12—P2—F7	89.3 (4)	C21—C20—H20	119.4
F11—P2—F7	90.2 (4)	C20—C21—C16	120.0 (5)
F10—P2—F8	90.1 (4)	C20—C21—H21	120.0
F12—P2—F8	90.3 (4)	C16—C21—H21	120.0
F11—P2—F8	178.5 (5)	O2—C22—C23	124.3 (4)
F7—P2—F8	88.7 (3)	O2—C22—C30	115.1 (3)
F10—P2—F9	89.2 (4)	C23—C22—C30	120.6 (4)
F12—P2—F9	179.6 (5)	C22—C23—C24	119.5 (5)
F11—P2—F9	89.7 (4)	C22—C23—H23	120.2
F7—P2—F9	90.6 (4)	C24—C23—H23	120.2
F8—P2—F9	89.4 (4)	C25—C24—C23	121.3 (5)

F7'—P2'—F8'	90.6 (8)	C25—C24—H24	119.3
F7'—P2'—F10'	179.2 (10)	C23—C24—H24	119.3
F8'—P2'—F10'	90.1 (8)	C24—C25—C26	120.3 (5)
F7'—P2'—F11'	91.6 (8)	C24—C25—H25	119.8
F8'—P2'—F11'	176.9 (10)	C26—C25—H25	119.8
F10'—P2'—F11'	87.6 (8)	C27—C26—C30	116.8 (4)
F7'—P2'—F12'	88.1 (9)	C27—C26—C25	123.7 (5)
F8'—P2'—F12'	90.9 (9)	C30—C26—C25	119.5 (5)
F10'—P2'—F12'	92.3 (9)	C28—C27—C26	120.7 (5)
F11'—P2'—F12'	91.3 (9)	C28—C27—H27	119.6
F7'—P2'—F9'	88.6 (8)	C26—C27—H27	119.6
F8'—P2'—F9'	89.3 (8)	C27—C28—C29	118.7 (5)
F10'—P2'—F9'	91.0 (9)	C27—C28—H28	120.6
F11'—P2'—F9'	88.7 (9)	C29—C28—H28	120.6
F12'—P2'—F9'	176.7 (10)	N6—C29—C28	122.9 (4)
C1—O1—C10	117.5 (4)	N6—C29—C32	116.6 (4)
C22—O2—C31	117.4 (4)	C28—C29—C32	120.4 (4)
C8—N1—C9	118.1 (4)	N6—C30—C26	122.0 (4)
C14—N2—C12	107.8 (4)	N6—C30—C22	119.4 (4)
C14—N2—C11	124.9 (3)	C26—C30—C22	118.6 (4)
C12—N2—C11	127.3 (4)	O2—C31—H31A	109.5
C14—N3—C13	108.3 (4)	O2—C31—H31B	109.5
C14—N3—C15	125.9 (4)	H31A—C31—H31B	109.5
C13—N3—C15	125.7 (4)	O2—C31—H31C	109.5
C35—N4—C34	107.9 (4)	H31A—C31—H31C	109.5
C35—N4—C36	125.9 (4)	H31B—C31—H31C	109.5
C34—N4—C36	126.2 (4)	N5—C32—C29	111.9 (3)
C35—N5—C33	107.9 (4)	N5—C32—H32A	109.2
C35—N5—C32	125.4 (4)	C29—C32—H32A	109.2
C33—N5—C32	126.7 (4)	N5—C32—H32B	109.2
C29—N6—C30	118.8 (3)	C29—C32—H32B	109.2
O1—C1—C2	124.8 (5)	H32A—C32—H32B	107.9
O1—C1—C9	115.4 (4)	C34—C33—N5	107.6 (4)
C2—C1—C9	119.8 (5)	C34—C33—H33	126.2
C1—C2—C3	119.7 (5)	N5—C33—H33	126.2
C1—C2—H2	120.1	C33—C34—N4	107.5 (4)
C3—C2—H2	120.1	C33—C34—H34	126.3
C4—C3—C2	121.9 (5)	N4—C34—H34	126.3
C4—C3—H3	119.1	N5—C35—N4	109.0 (4)
C2—C3—H3	119.1	N5—C35—H35	125.5
C3—C4—C5	120.5 (5)	N4—C35—H35	125.5
C3—C4—H4	119.8	N4—C36—C37	113.2 (4)
C5—C4—H4	119.8	N4—C36—H36A	108.9
C6—C5—C9	117.6 (4)	C37—C36—H36A	108.9
C6—C5—C4	122.8 (5)	N4—C36—H36B	108.9
C9—C5—C4	119.6 (5)	C37—C36—H36B	108.9
C7—C6—C5	119.5 (5)	H36A—C36—H36B	107.8
C7—C6—H6	120.2	C42—C37—C38	117.2 (5)
C5—C6—H6	120.2	C42—C37—C36	121.3 (5)

C6—C7—C8	118.8 (5)	C38—C37—C36	121.5 (5)
C6—C7—H7	120.6	C37—C38—C39	120.9 (5)
C8—C7—H7	120.6	C37—C38—H38	119.5
N1—C8—C7	123.7 (4)	C39—C38—H38	119.5
N1—C8—C11	116.7 (4)	C40—C39—C38	119.4 (6)
C7—C8—C11	119.6 (4)	C40—C39—H39	120.3
N1—C9—C5	122.2 (4)	C38—C39—H39	120.3
N1—C9—C1	119.2 (4)	C39—C40—C41	121.6 (6)
C5—C9—C1	118.5 (4)	C39—C40—H40	119.2
O1—C10—H10A	109.5	C41—C40—H40	119.2
O1—C10—H10B	109.5	C40—C41—C42	118.3 (6)
H10A—C10—H10B	109.5	C40—C41—H41	120.8
O1—C10—H10C	109.5	C42—C41—H41	120.8
H10A—C10—H10C	109.5	C37—C42—C41	122.6 (5)
H10B—C10—H10C	109.5	C37—C42—H42	118.7
N2—C11—C8	110.1 (3)	C41—C42—H42	118.7
C10—O1—C1—C2	−3.3 (9)	C31—O2—C22—C23	3.0 (6)
C10—O1—C1—C9	176.6 (6)	C31—O2—C22—C30	−177.4 (4)
O1—C1—C2—C3	179.6 (5)	O2—C22—C23—C24	179.0 (4)
C9—C1—C2—C3	−0.3 (8)	C30—C22—C23—C24	−0.6 (6)
C1—C2—C3—C4	−0.7 (10)	C22—C23—C24—C25	0.1 (7)
C2—C3—C4—C5	1.5 (10)	C23—C24—C25—C26	0.7 (8)
C3—C4—C5—C6	−179.8 (6)	C24—C25—C26—C27	179.0 (5)
C3—C4—C5—C9	−1.1 (8)	C24—C25—C26—C30	−1.1 (7)
C9—C5—C6—C7	0.3 (7)	C30—C26—C27—C28	0.2 (7)
C4—C5—C6—C7	179.0 (5)	C25—C26—C27—C28	−179.9 (5)
C5—C6—C7—C8	1.1 (8)	C26—C27—C28—C29	−2.1 (8)
C9—N1—C8—C7	1.6 (6)	C30—N6—C29—C28	−0.2 (6)
C9—N1—C8—C11	−177.1 (3)	C30—N6—C29—C32	−178.9 (3)
C6—C7—C8—N1	−2.2 (7)	C27—C28—C29—N6	2.1 (7)
C6—C7—C8—C11	176.4 (4)	C27—C28—C29—C32	−179.2 (4)
C8—N1—C9—C5	0.0 (6)	C29—N6—C30—C26	−1.8 (5)
C8—N1—C9—C1	−179.7 (4)	C29—N6—C30—C22	179.4 (3)
C6—C5—C9—N1	−0.9 (7)	C27—C26—C30—N6	1.8 (6)
C4—C5—C9—N1	−179.6 (4)	C25—C26—C30—N6	−178.1 (4)
C6—C5—C9—C1	178.8 (4)	C27—C26—C30—C22	−179.5 (4)
C4—C5—C9—C1	0.1 (7)	C25—C26—C30—C22	0.6 (6)
O1—C1—C9—N1	0.4 (6)	O2—C22—C30—N6	−0.6 (5)
C2—C1—C9—N1	−179.7 (4)	C23—C22—C30—N6	179.0 (3)
O1—C1—C9—C5	−179.3 (4)	O2—C22—C30—C26	−179.4 (3)
C2—C1—C9—C5	0.6 (7)	C23—C22—C30—C26	0.2 (5)
C14—N2—C11—C8	−105.6 (4)	C35—N5—C32—C29	−111.9 (4)
C12—N2—C11—C8	71.5 (5)	C33—N5—C32—C29	66.0 (6)
N1—C8—C11—N2	86.3 (4)	N6—C29—C32—N5	59.0 (5)
C7—C8—C11—N2	−92.4 (5)	C28—C29—C32—N5	−119.7 (4)
C14—N2—C12—C13	−0.2 (5)	C35—N5—C33—C34	−0.5 (5)
C11—N2—C12—C13	−177.7 (4)	C32—N5—C33—C34	−178.7 (4)
N2—C12—C13—N3	0.1 (5)	N5—C33—C34—N4	0.2 (5)
C14—N3—C13—C12	0.1 (5)	C35—N4—C34—C33	0.2 (5)

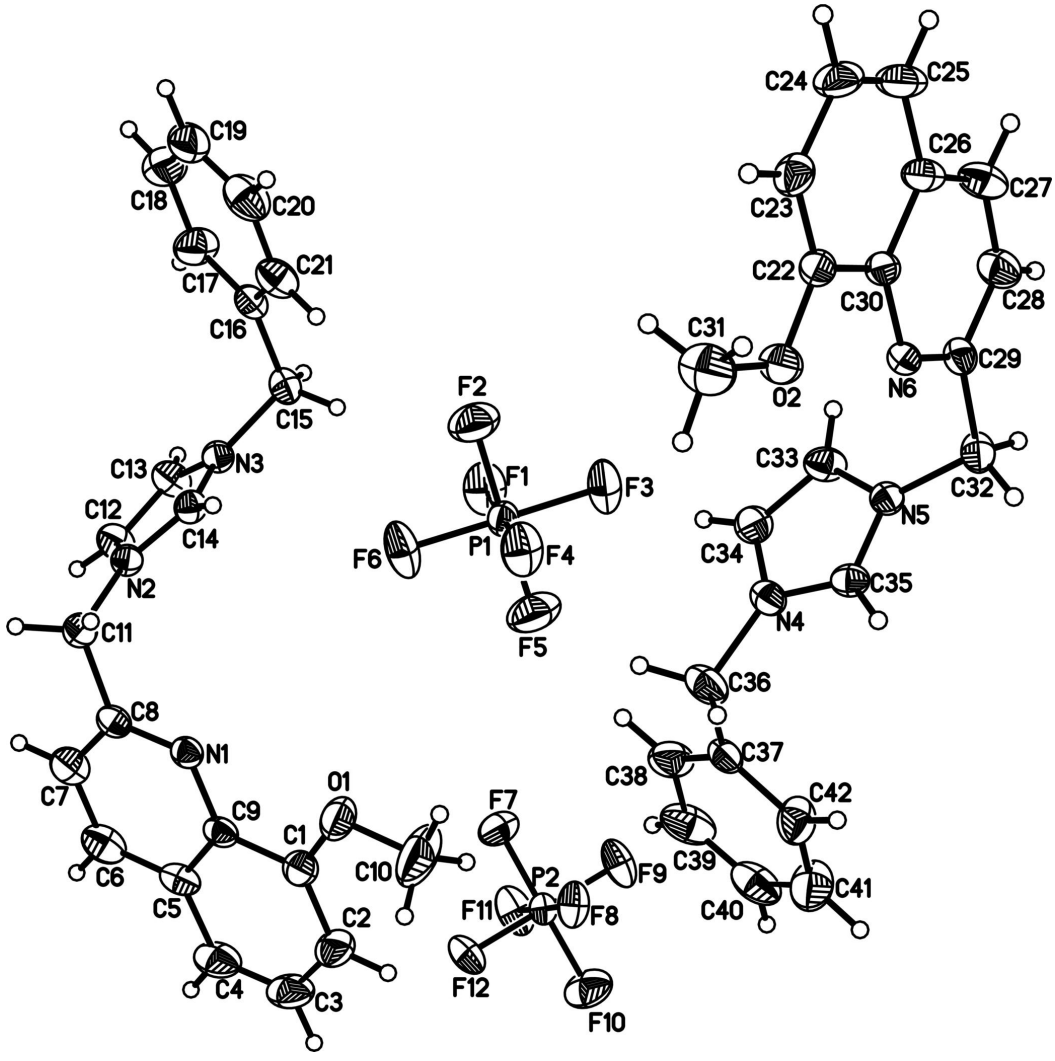
C15—N3—C13—C12	−177.3 (4)	C36—N4—C34—C33	−177.6 (4)
C13—N3—C14—N2	−0.2 (5)	C33—N5—C35—N4	0.6 (5)
C15—N3—C14—N2	177.1 (3)	C32—N5—C35—N4	178.9 (3)
C12—N2—C14—N3	0.3 (5)	C34—N4—C35—N5	−0.5 (5)
C11—N2—C14—N3	177.8 (3)	C36—N4—C35—N5	177.3 (4)
C14—N3—C15—C16	−74.3 (5)	C35—N4—C36—C37	−98.1 (5)
C13—N3—C15—C16	102.6 (5)	C34—N4—C36—C37	79.4 (6)
N3—C15—C16—C21	104.4 (5)	N4—C36—C37—C42	84.1 (6)
N3—C15—C16—C17	−77.1 (6)	N4—C36—C37—C38	−97.9 (6)
C21—C16—C17—C18	−0.4 (8)	C42—C37—C38—C39	−0.3 (8)
C15—C16—C17—C18	−178.9 (5)	C36—C37—C38—C39	−178.5 (5)
C16—C17—C18—C19	−1.1 (10)	C37—C38—C39—C40	0.2 (9)
C17—C18—C19—C20	2.7 (11)	C38—C39—C40—C41	0.7 (10)
C18—C19—C20—C21	−3.0 (10)	C39—C40—C41—C42	−1.5 (11)
C19—C20—C21—C16	1.5 (9)	C38—C37—C42—C41	−0.5 (9)
C17—C16—C21—C20	0.2 (8)	C36—C37—C42—C41	177.7 (6)
C15—C16—C21—C20	178.7 (5)	C40—C41—C42—C37	1.4 (11)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11B···F6^{i}	0.97	2.53	3.071 (7)	115
C12—H12···F9^{ii}	0.93	2.53	3.403 (11)	157
C13—H13···F9^{iii}	0.93	2.42	3.341 (11)	173
C14—H14···N1^{i}	0.93	2.38	3.248 (5)	156
C15—H15A···F11^{iii}	0.97	2.39	3.314 (8)	159
C35—H35···N6^{iv}	0.93	2.42	3.343 (5)	174
C36—H36A···F8^{v}	0.97	2.52	3.217 (8)	129

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) *x*+1, *y*, *z*; (iii) −*x*+1, −*y*+1, −*z*; (iv) −*x*+1, −*y*, −*z*+2; (v) −*x*+1, −*y*+1, −*z*+1.

Fig. 1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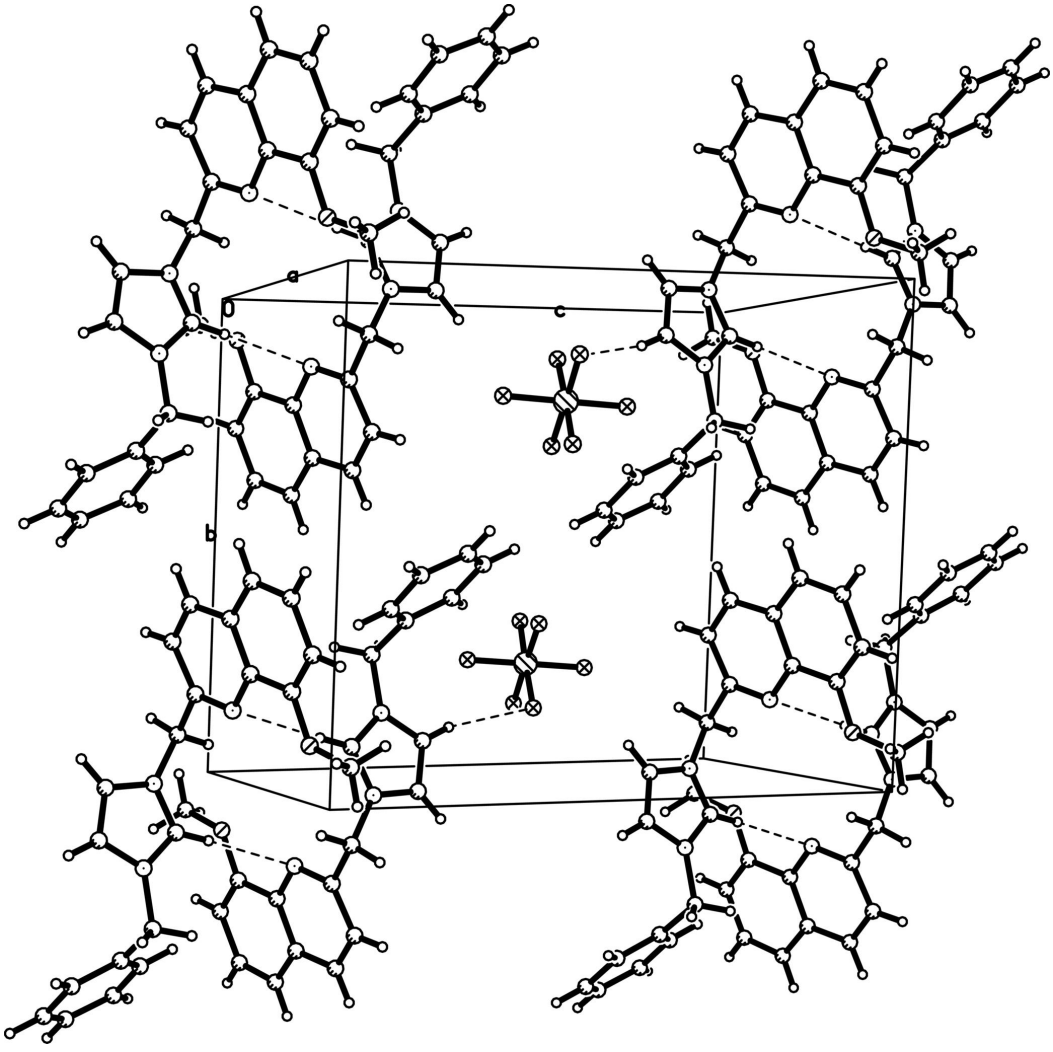
Fig. 2